# REPORT DOCUMENTATION PAGE

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| 1. AGENCY USE ONLY ( Leave Blank) | 2. REPORT DATE May 29, 2001 | 3. REPORT TYPE AND DATES COVERED<br>Final Report ~~1966 to Dec. 2000~~<br>01 Sep 96 - 30 Nov 00 |
|---|---|---|

| 4. TITLE AND SUBTITLE<br>Monte Carlo Studies of Continuous Hamiltonian Systems | 5. FUNDING NUMBERS<br>36151-ph-sr<br>DAAH04-93-D-0002 |
|---|---|
| 6. AUTHOR(S)<br>Mikael Ciftan and Robert G. Brown | |
| 7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)<br>Duke University, Durham, NC. | 8. PERFORMING ORGANIZATION REPORT NUMBER |
| 9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)<br>U. S. Army Research Office<br>P.O. Box 12211<br>Research Triangle Park, NC 27709-2211 | 10. SPONSORING / MONITORING AGENCY REPORT NUMBER<br>36151.6-PH-SR |

11. SUPPLEMENTARY NOTES
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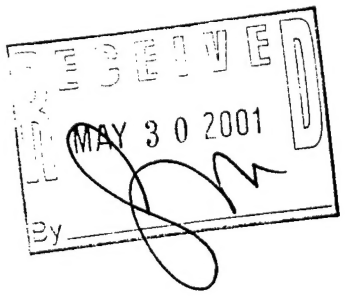


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13. ABSTRACT (Maximum 200 words)

Under this grant, three main categories of research was conducted, all related to the correlation problem in Theoretical physics that arises from Many-Body interactions in Quantum Physics or from the effects of Multiple Scattering on Coherence. We have studied the Heisenberg Ferromagnet (HF) both in its classical and quantum versions. New details were obtained in the finite-size scaling relations of the HF that are tied to the issue of spontaneous symmetry breaking and the formation of Goldstone massless bosons—this was carried out using the celebrated Monte Carlo formalism on the classical HF. For the calculation of the Partition Function (PF) of the Quantum form of the HF, we have derived a new Theorem we call " A Reduction Theorem" which substantially reduces the number of matrix elements that contribute to the PF. The Theorem is valid for any number of quantum HF spins. In particular we have also obtained closed analytical/algebraic expressions of the Partition Function of up to four Quantum Heisenberg Spins. This result can be applied to any number of spins on any finite lattice in an approximation scheme that is still being explored. In essence, both the classical and quantum methods are needed to resolve some outstanding issues regarding the critical exponents of the HF. The finite-size scaling relations are also relevant to the nanotechnology driven issues related to nano-sized magnetism. The correlation problem also arises in the case of electron correlations in Condensed Matter when the bonding between atoms shows a strong redistribution of bonding orbitals upon condensation and the insertion of "impurity" atoms into the system, such as the insertion of Hydrogen into Nickel Aluminides. This we also have studied and made a contribution to via our earlier work on band structure theory where we showed clearly that "the Full Potential" in the Wigner-Seitz Cell must be taken into account for correct prediction of materials properties. This has now become well accepted and has been adopted, even into the Density Functional Formalism, per force. On the coherence properties of radiation, we have demonstrated that we can use multiple scattering from specially engineered "roughened" surfaces to control the coherence properties of radiation. Though this work has been carried mostly by others, we were instrumental in directing the research into the particular aspects of "Coherence Control" because of our involvement in "Photon Correlation" in our earlier work under the previous grant. That work produced a first-principles derivation of Quantum Optics effects published circa September 89 in Physical Review A. It is clear that we have been investigating concrete examples of the correlation problem in order to learn from these and to make an eventual contribution to the "exchange-correlation" problem of Many-body Theoretical Physics.

| 14. SUBJECT TERMS | | | 15. NUMBER OF PAGES |
|---|---|---|---|
| | | | 16. PRICE CODE |
| 17. SECURITY CLASSIFICATION OF REPORT | 18. SECURITY CLASSIFICATION ON THIS PAGE | 19. SECURITY CLASSIFICATION OF ABSTRACT | 20. LIMITATION OF ABSTRACT |
| **UNCLASSIFIED** | **UNCLASSIFIED** | **UNCLASSIFIED** | **UL** |

NSN 7540-01-280-5500

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REPORT TITLE: Monte Carlo Studies of Continuous Hamiltonian Syustems

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SUBMITTED FOR PUBLICATION TO (applicable only if report is manuscript):

Mikael Ciftan

Sincerely,

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**Papers published under Grant No. 36151-PH-SR**

"High-precision evaluation of the static exponents of the classical Heisenberg Ferromagnet" (with R.G. Brown), *Physical Review Letters* 76, 1352, 1996.

"Observation of Giant Enhanced Backscattering of Light from Weakly Rough Dielectric Films on Reflecting Metal substrates." *Optical Engineering*, 35, 370, 1996.

"First-principles determination of the effects of Boron and Sulfur on the ideal Cleavage Fracture in $Ni_3Al$." with S. Sun, N. Kioussis, A. Gonis, Mat. Res. Soc. Symp. Proc. 409, 183 (1996).

"Effects of Boron and Sulfur on the Ideal Yield Stress of $Ni_3Al$," S. Sun, N. Kioussis, M. Ciftan, and A. Gonis, NATO, ASI Series, **355**, 413 (1996).

"Critical exponents of the classical Heisenberg ferromagnet," Robert G. Brown and Mikeal Ciftan, Phys. Rev. Lett. 76, 1352 (1996).

"Critical Scaling of the dynamical critical expeonents of the classical Heisenberg Ferromaqgnet." Robert G. Brown and Mikael Ciftan, Phys. Rev. B54, 15860 (1996).

"The Dynamic Critical Exponents of the 3d, O(3) Classical Heisenberg Model". R. G. Brown and M. Ciftan, in Condensed Matter Theories 10, ed. Artur Pols, Nova Science Publishers, New York, 1996. Also presented as invited talk at Condensed Matter Theories Workshop 19.

"Critical exponents of the Classical Heisenberg Model, Robert G. Brown and Mikael Ciftan, paper presented at Condensed Matter Theories Workshop 20, in Pune, India in December 1996; and published in the conference proceedings book: Condensed Matter Theories 12, ed. John W. Clark and P. V. Panat, Nova Science Pub., 1997.

Brown and Ciftan reply, Robert G. Brown and Mikael Ciftan: Reply to a Comment on "Critical exponents of the classical Heisenberg Ferromagnet" by C. Holm and W. Janke, Phys. Rev. Let. 78, 2266 (March 17, 1997).

" Mo0nte Carlo Evaluation of the Helicity Modulus of the O(3) Heisenberg m Model:. R. G. Brown and M. Ciftan, in Condensed Matter Theories 13, ed. D. Ernst and John W. Clark, Nova Science Pulishers, 1999; also presented as invited talk at Condensed Matter Theories Workshop 22.

Invited talk at the MRS Fall 1997 meeting: Effect of Hydrogen on the _5 (210) grain boundary of $Ni_3Al$: A first principles study by N. Kioussis, Gang Lu, R. Wu and M.Ciftan.

"First-principles studies of Sigma-5 tilt grain boundary in Ni3Al," Gang Lu, N. Kioussis, R. Wu and M. Ciftan. Phys. Rev. B 59, 891 (1999).

"Rough Surface enhanced scattering" with Zu-Han Gu, Z. Q. Lin, SPIE Conference 3426, July 1998.

"Coherence from Rough Surface Scattering,"b with Zu-Han Gu and Jun Q. Lu, in "Recent Research Developments in Optical Engineering,"pp. 161-212, 2 (1999).

"Effect of Hydrogen on Grain-Boundary Embrittlement," with N. Kioussis, Gang Lu, and R. Wu, presented at the condensed Matter Theories Workshop in Ithaki, 1999; Condensed Matter Theories, p.313, Vol. 15, Ed.s: G. S. Anagnostatos et al. Nova Science Publishers, N.Y., 2000.

"A study of the critical exponents of the Helicity Modulus of the O(3) Heisenberg Model," with R. Brown.

presented at the condensed Matter Theories Workshop in Ithaki, 1999:
Condensed Matter Theories, p.77, Vol. 15, Ed.s: G. S. Anagnostatos et al. Nova Science Publishers, N.Y., 2000.

"Coherence and Fluctuation of Light from Rough Surface Scattering" with Zu-Han Gu and Jun Q. Lu, in Frontiers of Laser physics and Quantum Optics, Edited by: Zhizhan Xu, Shengwu Xie, Shi-Yao Zhu and Marlan O. Scully, Springer-Verlag, New York 2000.

"Non-linear dynamics of a driven inhomogeneous plasma oscillator," with P. Bakshi and K. Kempa, presented as an invited talk at the March 2000 meeting of the American Physical Society.

Invited talk "From "Metallurgy and Ceramics" to "Materials Science" – a personal perspective," to the 2000 TMS (The Metals and materials Society) Fall Meeting, Oct. 8-12, 2000, in St. Louis, MO. Published in "The Science of Alloys for the 21st Century." Ed.s: by Patrice E. A. Turchi, Robert D. Shull and Antonios Gonis, TMS Publications, 2000.

"Enhanced Backscattering at Grazing Angle" with Zu-Han Gu, submitted to SPIE-2001 Annual Meeting, Conference-AM423, San Diego.

**Book:**

Electron Correlations and Materials Properties, Eds.: A. Gonis, N. Kioussis and M. Ciftan, Kluwer Academic Plenum Publishers, 1999.

**Papers that have been in preparation under this grant:**

"The Critical Scaling and the Helicity Modulus for the Classical Heisenberg Model" with R. G. Brown, submitted to Phys. Rev. Letters, June 2000, being updated with additional data.

"A Theorem on the Partition Function of Finite Number of Heisenberg Spins" to be submitted to Journal of Mathematical Physics.

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**Extended Discussion of Results**

We have completed work on the Heisenberg Ferromagnet (HF) wrt its static and critical exponents. This work is probably the highest precision work completed to date on these critical exponents obtained using the Monte Carlo method. In order to arrive at this juncture we had to improve the very Monte Carlo techniques themselves, meanwhile making a contribution also to the statistical sampling methodologies-- which in and of itself is of value to sampling techniques. In order to resolve issues related to the finite-size scaling of these critical exponents, which has persisted to this date, we finally had to focus on Fisher's Helicity Modulus for the HF which determines spin-wave stiffness as perhaps "the" key single parameter that characterizes the symmetry breaking that occurs at the critical temperature and consequently the appearance of Goldstone (massless) bosonic modes.

For the last year and a half we have been conducting these high-precision calculations but the computational methodology is necessarily slow due to the three dimensional characteristics of the spins and the complexity of the steps in the calculations. Although we had gone to much larger size lattices than usual, the referee of our paper submitted to Phys. Rev. Letters, Prof. M. Fisher, has suggested that we go even further into larger sizes, 64X64X64 or higher number of spins, to obtain further data to substantiate our conclusions. This has required us to tool up our computational hardware substantially. Prof. Fisher suggested this in order that we improve further our finite size scaling fits which differ somewhat from earlier theoretical predictions but appear consistent with the very latest results from Renormalization Group Theory methods. Therefore, it was quite important to go forward with this retooling of our already very comprehensive computational infrastructure.

Fortunately, one of us is an acknowledged expert in "Cluster Computing" and thus with minimum of funding we have been able to start to upgrade our computational apparatus substantially to achieve this goal.

We are currently just completing the first-phase construction of this computational resource designed to help us address this problem at the requisite lattice sizes and degrees of accuracy. This resource will be augmented at least twice more during the life of this grant, which should give us the resources required to properly complete this project and publish our interesting results.

We have also derived a new algebraic expression of the Partition Function (PF) of the Quantum HF for up to four spins. This provides an exact closed form expression of the PF that is in reduced computational form because of a new Theorem we have proven regarding the matrix elements that enter the calculation of the PF. This theorem has general validity regardless of the number of spins involved. Its application to more than four HF spins still awaits further research. We have made conjectures on approximation schemes that will be explored. If a valid approximation schemes is found, that will give us an independent way of checking the finite size scaling relations of the critical exponents of the HF.

Earlier in our research we had developed a self-consistent non-muffin-tin band structure theory for the calculation of the electronic energy level of crystalline solids. We had tested it and found to be rather powerful in that it should be able to treat such condensed matter systems as GaAs or tetrahedrally coordinated semiconductors where the electronic cloud between atoms do show high density; for such cases, the muffin-tin approximation is not valid and cannot be used in a self-coinsistent loop of calculations. Thus we had improved upon the celebrated KKR (Korringa-Kohn-Rostocker) theory. This was well explored at a Materials Science Symposium in Boston over several days; one conclusion was that one should make every effort to take into account fully the whole of the atomic potential in the Wigner-Seitz cell. That is, not to truncate the atomic potential into a spherical muffin-tin part within the Wigner-Seitz cell, throwing away the rest between the Muffin-tin regions of the atoms. This then has become the "Full Potential" approach now well adopted. With a colleague we have since published papers showing explicitly this point, that unless the full potential is taken into account, some essential features of materials are lost-- calculations do not agree with experimental results. This becomes particularly serious when one deals with hydrogen embrittlement, for example, say in Nickel Aluminides. When the electron correlations are thus self-consistently taken into account, then calculated properties such as cleavage energies, of defect bearing structures, even complicated ones such as grain boundaries and stacking fault energies all agree well with observed data. First principles self consistently calculated parameters can then go safely into semi-classical formulations such as the Peirls-Nabarro formalism for stacking fault energies. The full potential is introduced into the Density Functional Formalism, per force.

Based on such successes, we now have gone back and are trying to upgrade our band structure calculation codes derived from our theory so that the scientific public will have full access to it via the Internet. Let us give some further details below, in the context of our publications.

We spent a great deal of effort during the period of 1980-1990 on band structure theory stemming from the Ph.D. Thesis of Prof. Robert G. Brown from Duke University, developing this "Generalized Non-muffin-tin Theory". See, for example, papers by R. G. Brown and M. Ciftan: Phys. Rev. B27, 4564 (1983); "Numerical tests of high precision multiple-scattering band theory," Phys. Rev. B33, 7937 (1986); "Multipolar Expansions for Multiple Scattering Theory," presented at the 1991 Materials Research Society Fall Symposium (session V) in Boston, MA and published in the symposium proceedings, among many others. In the last work, in particular, we proved beyond any doubt that the true non-muffin-tin solutions exist and are unconditionally convergent in our multiple scattering approach and no other.

The confluence of these two lines of research were therefore very fortuitous, and we deemed the time appropriate for returning to the implementation of our exact band theory in a full self-consistent-field calculation. For the last six months considerable effort has been expended porting our old band theory Fortran code to C, installing modern numerical methods and libraries in place of the old, rewriting

the routines for generating the structure constants of multiple scattering band theory from scratch to take advantage of the considerable improvements in methodology that had occurred since our original publications. and parallelizing parts of the code to take efficient advantage of the "beowulf" computational resource being built to also conduct our Monte Carlo researches into the Helicity Modulus.
Effort is also being expended to ensure that the resulting code is optimally portable -- it is being written free from the use of proprietary libraries so it can be openly distributed on the web to any who might care to use it in the many venues of physics and engineering where high-precision band structure or crystal potentials are needed.

At this time the band structure computation code's status is that the C port is approximately half finished -- the structure constant routines work and effort is being expended on the requisite integrations of coupled ordinary differential equations and potential decompositions. We hope to have a working revision completed by the end of the summer. In the meantime, we expect to resume our Monte Carlo computations within the next two to three week and should keep our computational resources fully busy at nearly 100% duty cycle from that point on to drive the Helicity Modulus project on to its conclusion.

Up to this point in this report we have discussed two of the three subject areas we outlined in the Abstract to this report. namely first the highly correlated phase transition phenomena of the Heisenberg Ferromagnet – spin systems. and secondly the electron correlations details that enter electronic band structure and materials properties of condensed matter systems. The electronic band structure was developed for systems at zero temperature (namely no Molecular Dynamics) and in order to better understand and formulate a theory at finite temperature (as compared to Molecular Dynamics approaches), we had delved into thermodynamic phase transition phenomena and thus worked first on the Ising spins and later have developed a methodology for the HF which should better represent the behavior of magnetic systems at finite temperatures. But then why were we also involved, right after R. G. Brown received his Ph.D. degree, together with him on Quantum Optics? To the outsider. this may appear rather arbitrary. However, the quantum optics system of a collection of two-level atoms was the perfect system to study the "Radiation Bath" without getting into the more difficult Thermodynamic Temperature Bath – which we finally have been tackling with our HF thrust. At that time we did make a good choice and we were able to derive *ab intio* from first principles a theory where with proper formulation of "correlation" between the two level atoms that gave us most of the then known quantum optics effects such as Optical Bistability, Photon Echo. Supperradiance. Significantly. we also had found an *anzatz* that worked for us in performing Quantum Demolition.

Now it was in that context that we had come to appreciate the connection between multiple scattering techniques of our band theory and photon correlations in quantum optics. Perhaps we could visit some remarkable coherence effects that one of us had been exposed to in his endeavors with Dr. Edward Collett and Prof. Emil Wolf who had devised a theory for the control of coherence. When finally the celebrated Universal Conductance Fluctuations was discovered. and the confluence of this condensed matter physics phenomenon with its counterpart in Optics became clear. one of us pursued this line and did contribute to research on scattering of light from surfaces whose roughness-characterizing statistical moments could be designed -- to produce such remarkable coherence control effects as the controlled retro-reflection of light scattered from these surfaces. That is why you see a number of publications in optics in the listing of publications provided.

In conclusion. we have demonstrated effects of correlations in spin systems. in electronic systems. and in photonic systems. We have seen these effects as high order correlations, localization v.s. delocalization. whether it was spins forming clusters near the phase transition temperature and their breakup due to the thermodynamic bath, the correlation of electronic orbitals joining atoms into molecular-like orbitals localized by inserted impurities such as hydrogen. or the correlations of photons to various orders forming partial coherence or the break-up of such due to thebdegree of randomness introduced on roughed surfaces in specific ways.
Thus we have been studying the role of correlations in Theoretical Physics.